Work in the Stockroom!

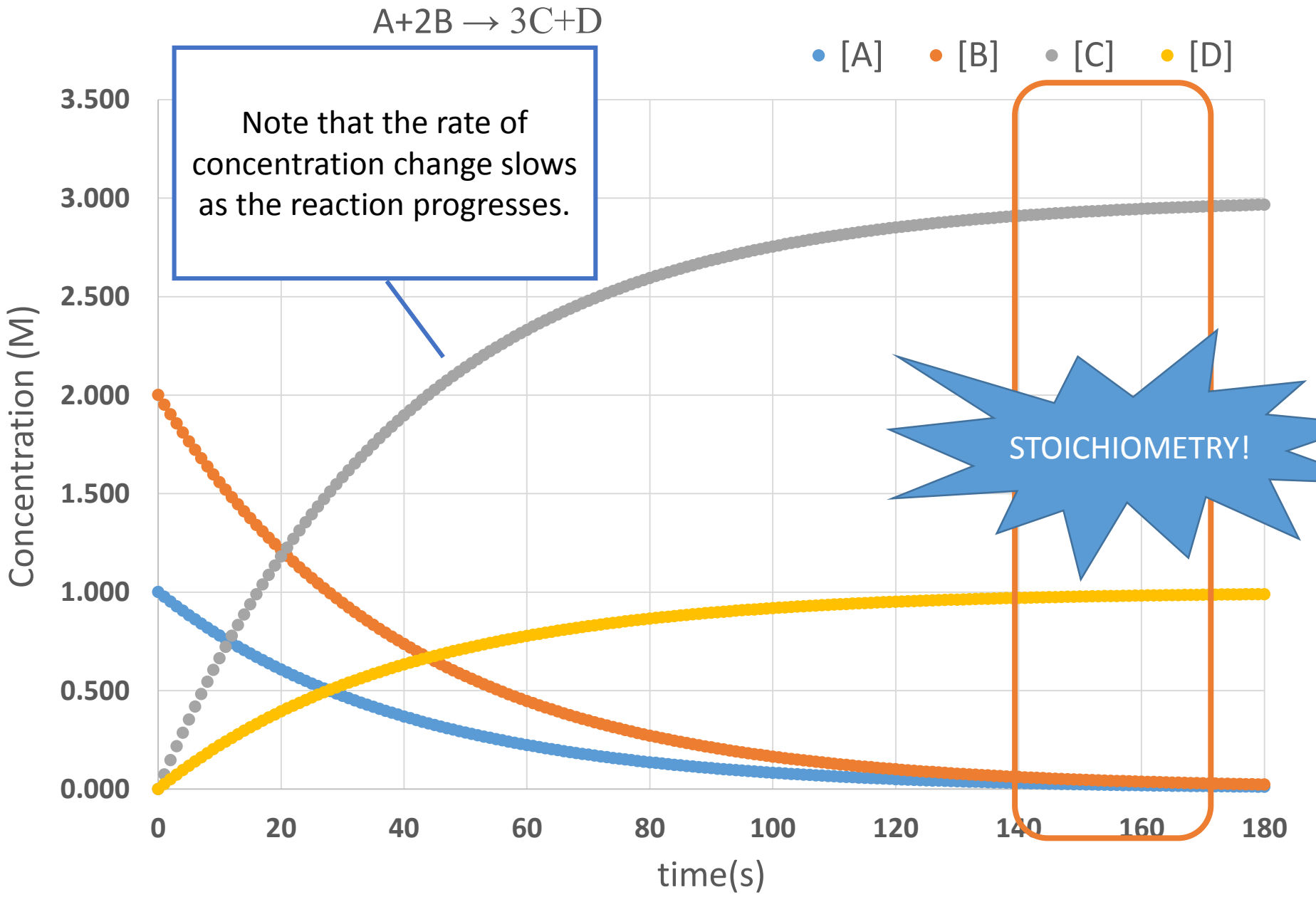
Completion of the following classes is required:

- CHEM 1450 College Chemistry I
- CHEM 1451 College Chemistry II
- CHEM 2401 Organic Chemistry I
- One four- or five-hour upper-division chemistry class

Chapter 20

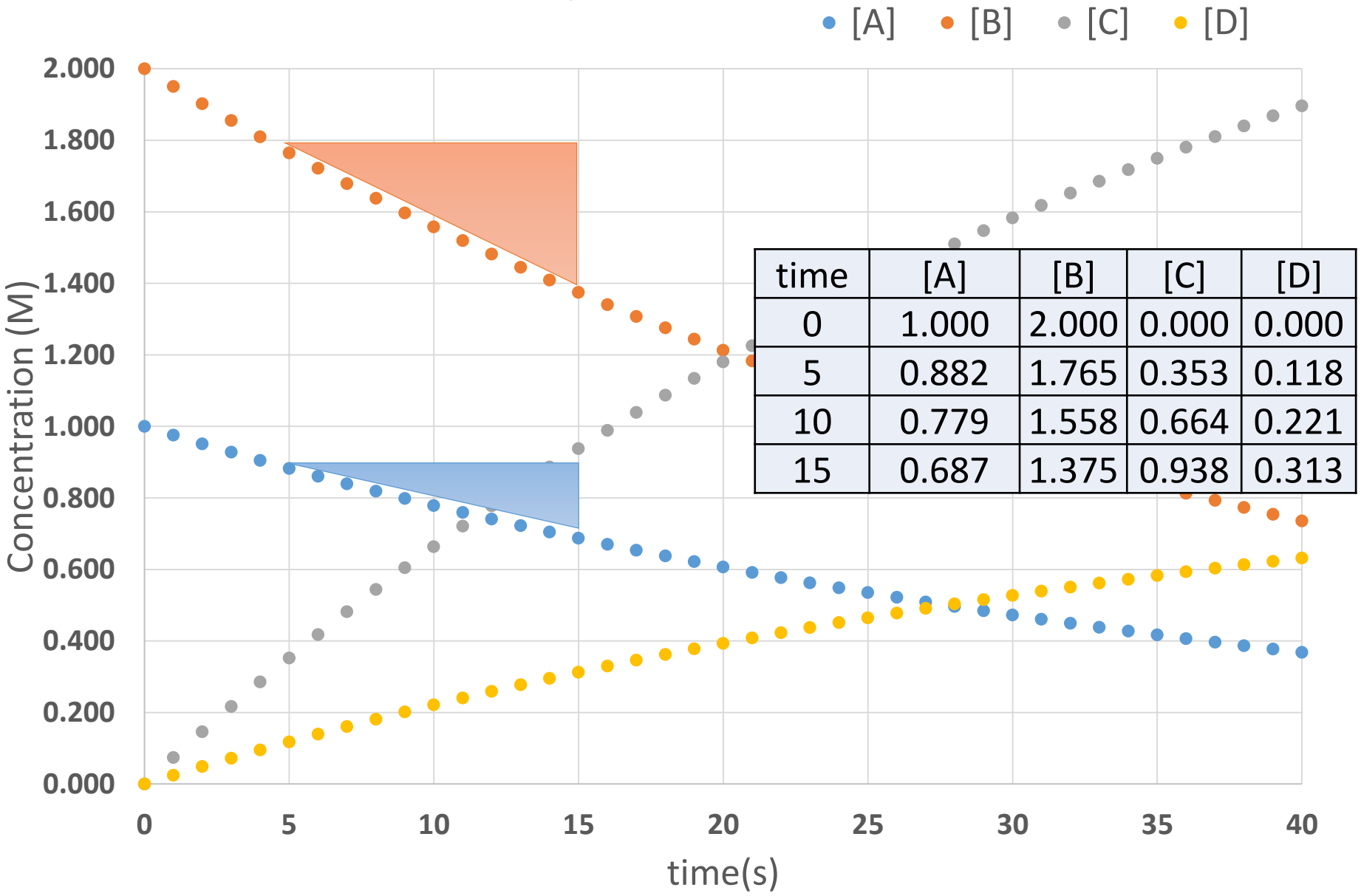
Kinetics

Time dependence of component concentration for the reaction:



Time dependence of component concentration for the reaction:

$$A + 2B \rightarrow 3C + D$$



time	[A]	[B]	[C]	[D]
0	1.000	2.000	0.000	0.000
5	0.882	1.765	0.353	0.118
10	0.779	1.558	0.664	0.221
15	0.687	1.375	0.938	0.313

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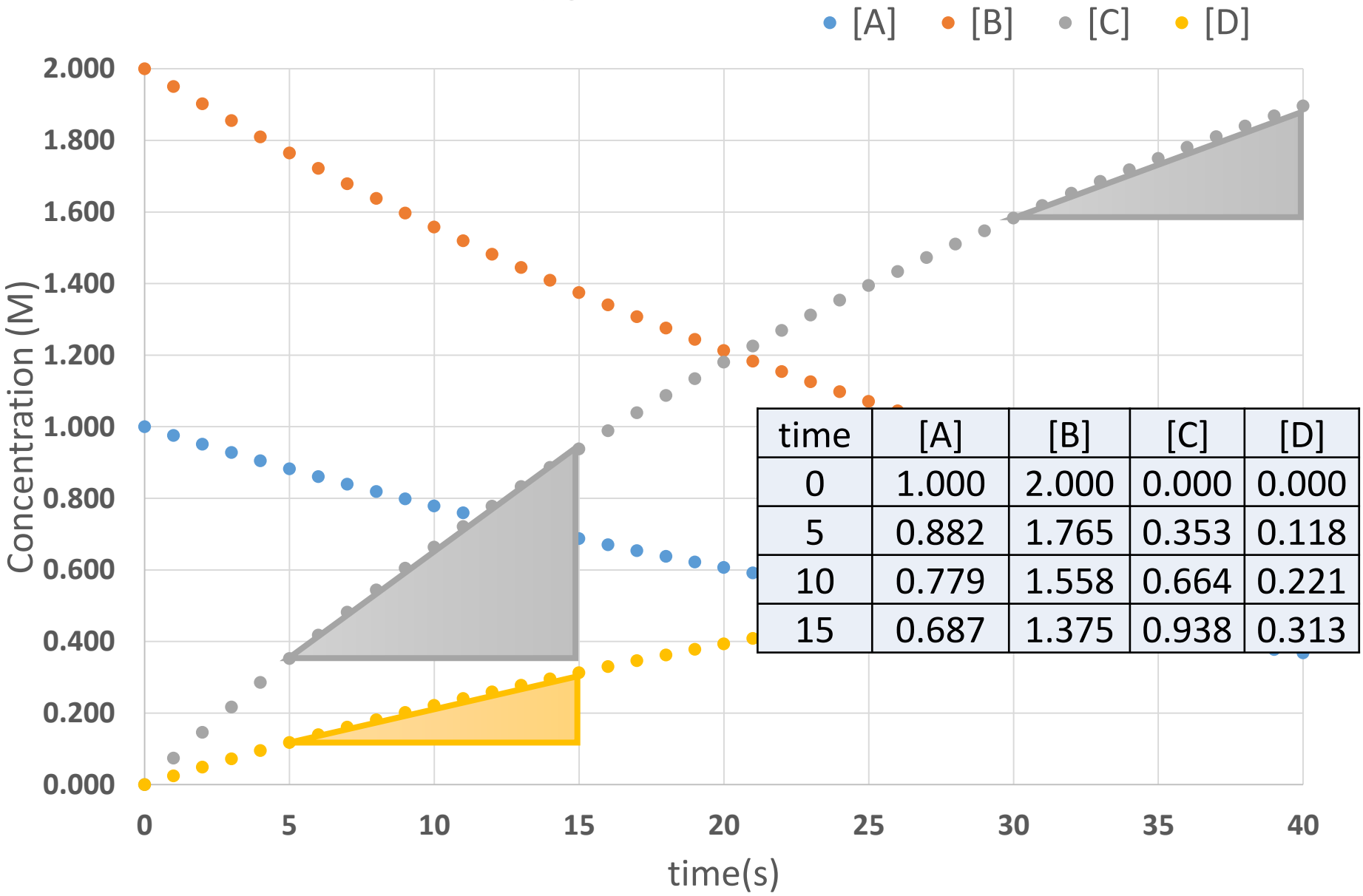

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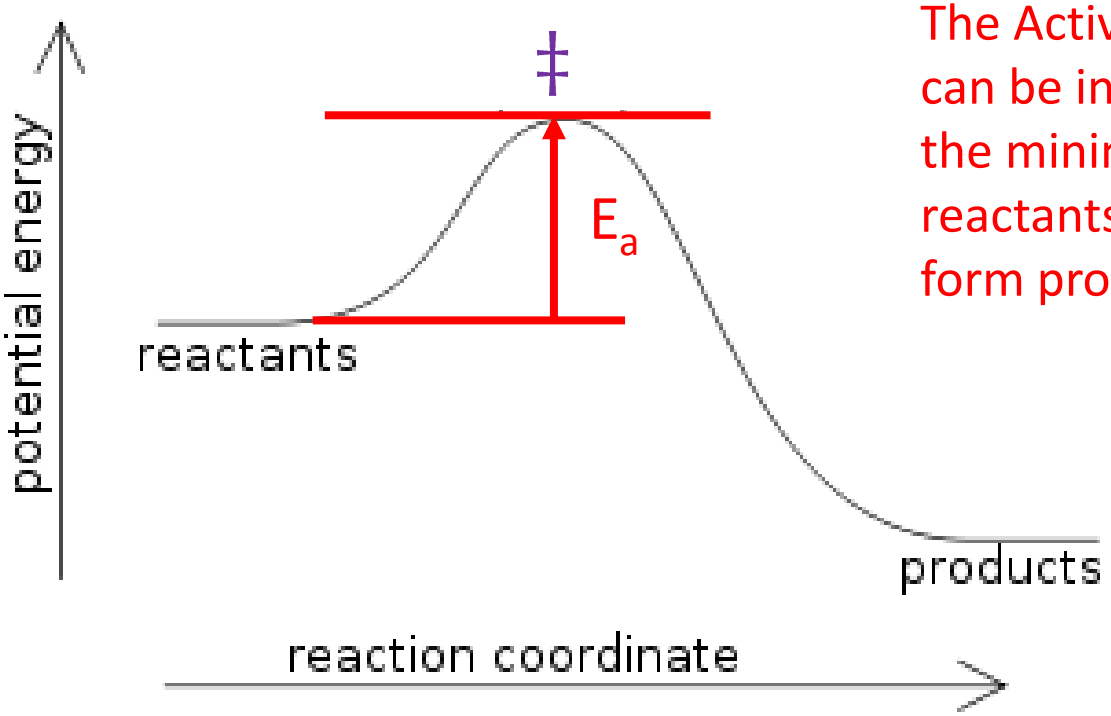
Integrated Rate Laws

Reaction Coordinate Diagram

The Activated complex corresponds to the geometry that is near the maximum potential energy.



The Activation Energy can be interpreted as the minimum energy reactants must have to form products.

The reaction coordinate summarizes all of the motions that are directly involved with forming products from reactants

Arrhenius Parameters

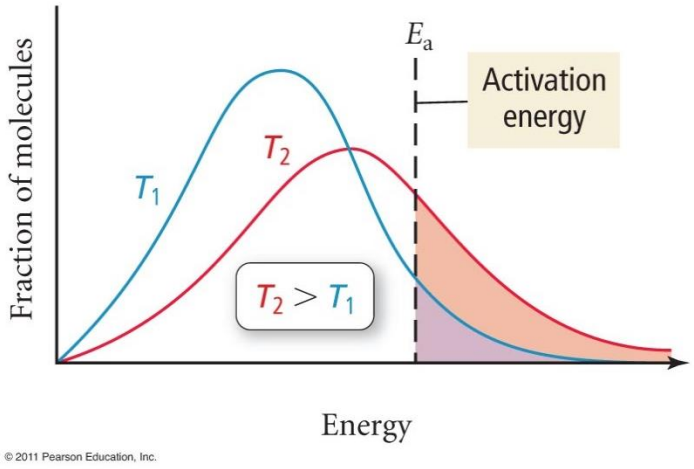
$$k = A \cdot e^{\frac{-E_a}{RT}}$$

Frequency Factor

Exponential Factor

$$A = p \cdot z$$

- Orientation Factor: “p”
  - the fraction of collisions that are actually successful due to colliding in the correct way.
  - NOT temperature dependent!
- Collision frequency: “z”
  - The number of collisions per unit time. Can be calculated.
  - Temperature dependent!



1st-Order Reversible Reactions

GOAL: To look at the connection between the rate constant and the equilibrium constant for a simple reversible process:

$$\boldsymbol{A \rightleftharpoons B}$$

$\boldsymbol{A \rightarrow B}$ Rate Constant= k_1 Rate Law: $\boldsymbol{v_1 = k_1[A]}$

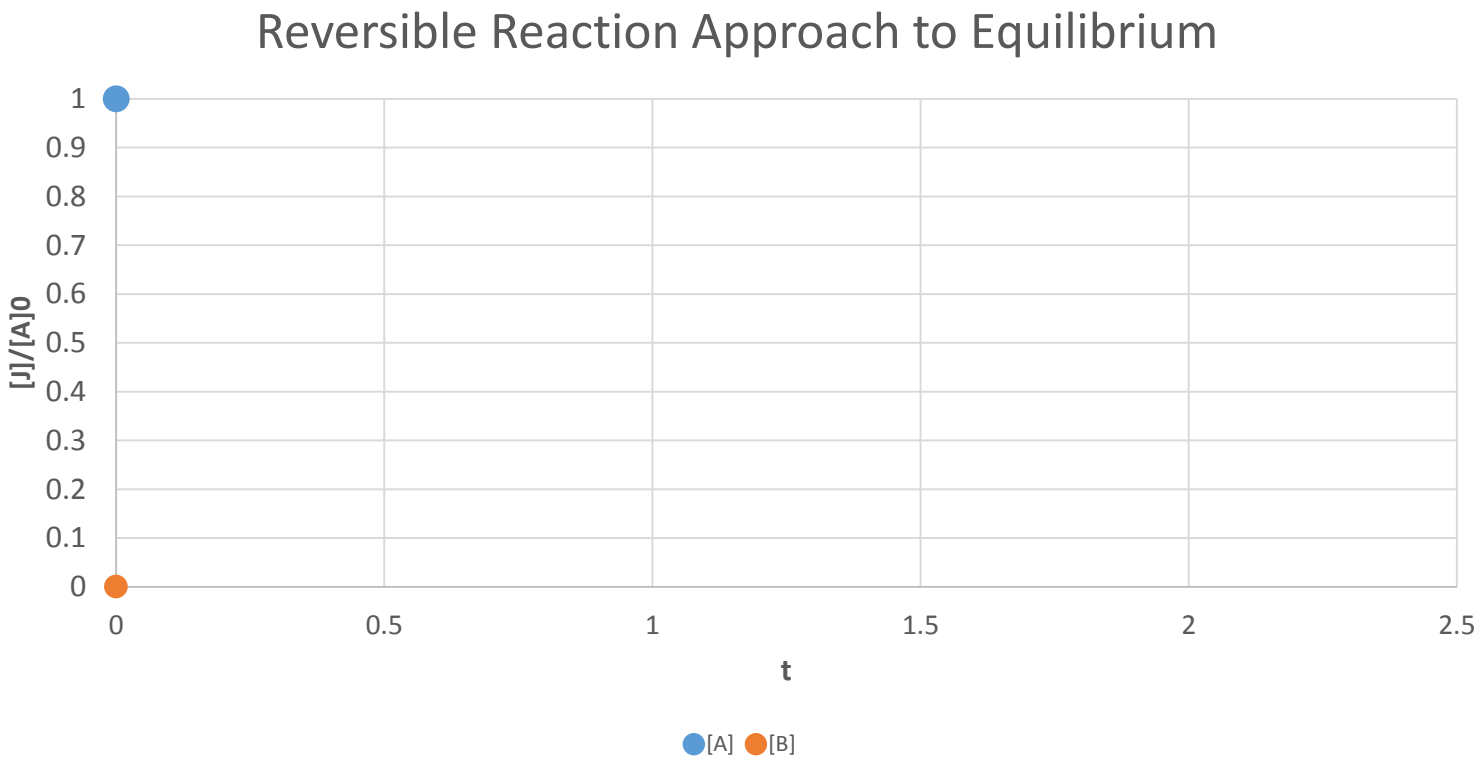
$\boldsymbol{B \rightarrow A}$ Rate Constant= k_{-1} Rate Law: $\boldsymbol{v_{-1} = k_{-1}[B]}$

The rate of change of A is dependent on both overall rates:

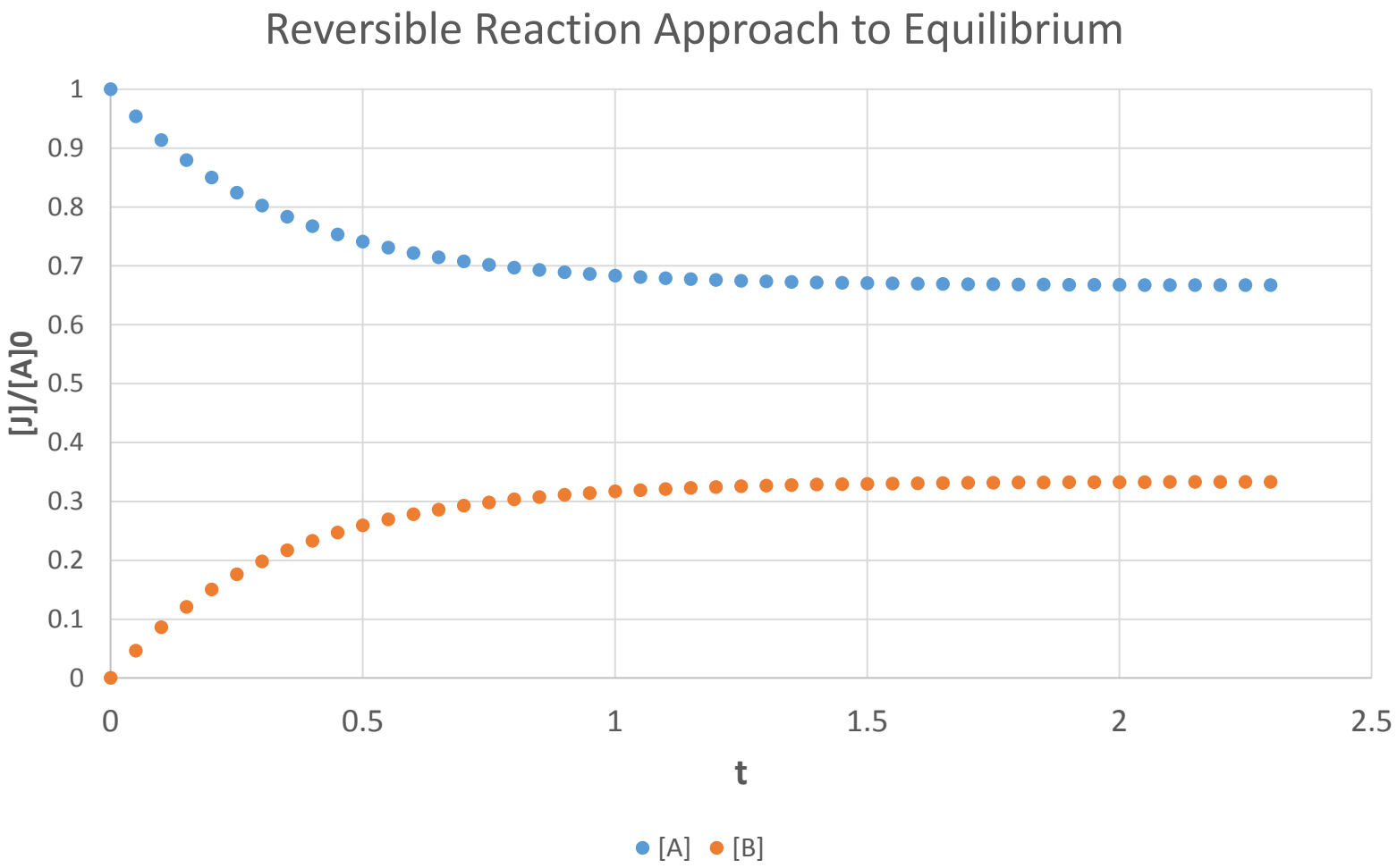
$$\frac{\boldsymbol{d[A]}}{\boldsymbol{dt}} = \boldsymbol{-k_1[A] + k_{-1}[B]}$$

Where are we at t = 0?

Assume that at t=0, $[A] = [A]_0$ and $[B] = 0$



As [A] and [B] approach Equilibrium:



Elementary Reactions

- **Reaction Order**: empirical quality
- **Molecularity**: The number of molecules that must collide for a reaction in an elementary reaction

- If you know the molecularity, you can deduce the order.
- If you know the order, you cannot assume you are talking about an elementary reaction OR that you know the molecularity.

Parallel Reactions

Assume that at t=0, there are NO Products, only Reactant

- The Branching Ratio is time independent!

- No matter what the ratios of rate constants are for a branch, the fraction of product concentration remains the same for all time.